REFINING AND END USE STUDY OF COAL LIQUIDS
TEST FUEL PRODUCTION AND TESTING - PART I

Cliff Lowe
cmlowe@bechtel.com
(415) 768-2513, (415) 768-2743 fax
Bechtel National, Inc.
P.O. Box 193965
San Francisco, CA 94119-3965

Jimell Erwin
jerwin@swri.edu
(210) 522-2389, (210) 522-5720 fax
Southwest Research Institute
P.O. Box 28510
San Antonio, TX 78228-0510

D. Stan Moulton
smoulton@swri.edu
(210) 522-3504, (210) 522-5720 fax
Southwest Research Institute
P.O. Box 28510
San Antonio, TX 78228-0510

1. Introduction

Bechtel National Inc., with Southwest Research Institute, Amoco Corporation, and the M. W. Kellogg Company as subcontractors, are conducting a study for DOE's Federal Energy Technology Center to determine the most cost effective combination of upgrading processes needed to make high quality, liquid transportation fuels from petroleum crude and direct and indirect coal liquefaction products in an existing petroleum refinery. This is a multi-faceted study which has been previously described.[1]

One key objective is to determine the most economical way of integrating coal liquefaction products into existing petroleum refineries to produce transportation fuels meeting future, e.g. year 2000 and beyond, Clean Air Act Amendments (CAAA) standards. An integral part of this objective is to produce, test, and compare these fuels with appropriate ASTM fuels. The comparison includes engine tests for compliance with the CAAA and other applicable fuel quality and performance standards.

Another objective involves a detailed economic evaluation of the costs of coprocessing the coal liquids to their optimum products. This study will reflect the cost of operations using state of the art refinery technology without allowing for the construction of new refineries. Some refinery modifications or additions may be included if they are economically justified. Economy of scale considerations in the coal liquefaction plant will influence the minimum amount of coal liquids that should be processed in the refinery.

Part I of this paper summarizes the production of transportation fuels that are blends of petroleum materials and direct coal liquids. The engine performance and emission testing of these fuels is reviewed in Part II of this paper.

2. Background

The original scope for this study called for testing three coal liquids: two direct liquids, POC-1/DL1 and POC-2/DL2 produced by Hydrocarbon Technologies, Inc, and a Fischer-Tropsch indirect liquid, IL1. Because of difficulties in the pilot plant testing, the scope for the DL1 liquid testing has been reduced in scope.

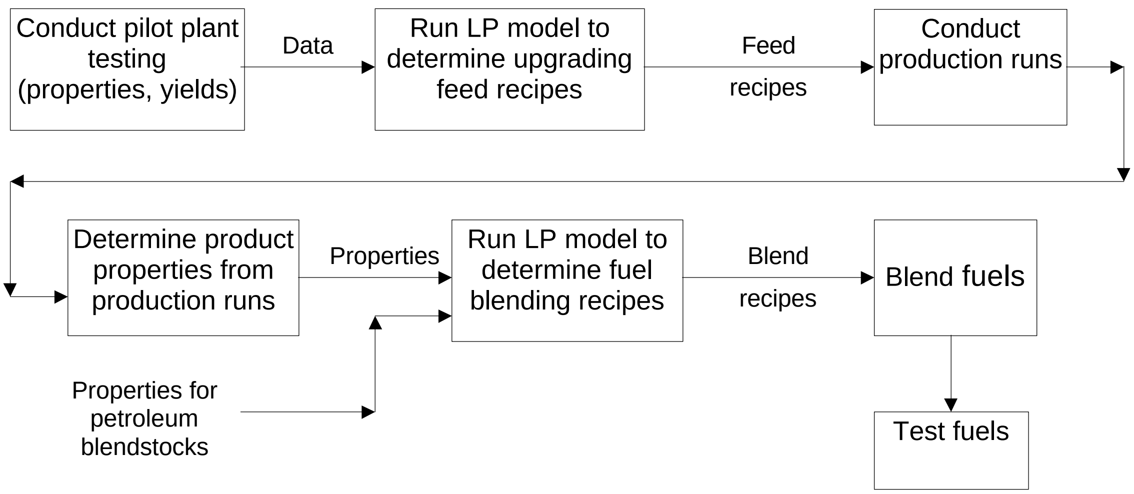
Because the IL1 materials required pre-processing (catalyst removal), the direct liquids were the initial objects of the fuel testing and testing of the IL1 material has been held postponed. Testing of Fischer-Tropsch liquids from commercial vendors of FT technology has been substituted.

For the DL2 liquid, there were five fuels tested: conventional regular gasoline, reformulated premium gasoline, Jet A, off-road diesel, highway diesel. For the DL1 liquid, there was a single fuel tested: highway diesel.

[1] Lowe, C. and S. Tam, "Refining and End Use Study of Coal Liquids," Proceedings of the Coal Liquefaction and Gas Conversion Contractors Review Conference, Pittsburgh, Sept. 7-8, 1994.

3. Fuel Production

The plan for the production of the fuels was a multi-step, interactive process between testing and linear programming (LP) analysis. Test data on neat coal liquid properties, upgrading yields, and product properties was used to first determine the composition of the feed to each production run, and then the fuel blending recipes. The following diagram is a schematic of the process used to develop the recipes:



3.1 Collect Characterization and Upgrading Data

The characterization work provided property data on the four fractions (light naphtha, medium naphtha, light distillate and heavy distillate) from each of the two direct coal liquids. Data on coal liquid upgrading yields and product properties was obtained from the pilot plant testing. Data for petroleum based streams was initially based on LP library data. In some instances, petroleum yields and product properties were based on data obtained during the first phase (petroleum feed) of each pilot plant run.

3.2 Determine Production Run Feed Compositions

The Process Industry Modeling System (PIMS) linear programming refinery model[2] was used to determine:

- The composition of the feed to each upgrading production run
- The blending recipes for each of the transportation fuels that will be tested

The key design bases for the model were:

- Product slates were based on projected year 2000 market demands based on a DOE-Energy Information Administration report[3]. Gasoline product specifications were based on EPA year 2000 guidelines and the Complex Emission Model. Jet and diesel specifications were based on estimates of future requirements. See Tables 1 - 3.

- Coal liquid/petroleum crude refinery feed ratio - Previous analyses have shown that there is no economic optimum amount of coal liquid that should be processed by the refinery. In all scenarios, as the amount of coal liquid increases, the value of the coal liquid (on a per barrel basis) steadily decreases. In other words, each additional barrel of coal liquid is more costly to process because of constraints of unit capacities, specifications, utilities, etc. It should be noted, however, that the high quality of both the DL1 and the DL2

---

[2] Lowe, C. and S. Tam, “Refining and End Use Study of Coal Liquids,” Proceedings of the Coal Liquefaction and Gas Conversion Contractors Review Conference, Pittsburgh, Sept. 7-8, 1994.
[3] Supplement to the Annual Energy Outlook 1995, DOE/EIA-0554(95), February, 1995

liquids (low heteroatom content, high hydrogen content, low end point) have resulted in estimated values that are higher than the base petroleum crude[4].

Since there is no optimum amount of coal liquid for processing, the coal liquid/petroleum crude refinery feed ratio was based on determining the maximum amount of coal liquid that an existing refinery can process. In this scenario, the refinery produces approximately 150,000 barrels per day of products. Unit expansion is not required or allowed. Coal liquid (at zero value) is allowed to replace as much of the petroleum crude as possible while still meeting the fixed product slate and volumes.

3.2.1 LP run to determine fuel production run feed compositions

For the above criteria the model was run to determine the composition of the feed for the various production runs. The refinery feed composition was as follows:

	DL1 feed	DL2 feed
PADD II crude mix, vol%	49.9	50.9
Coal liquid, vol%	37.5	37.0
MTBE, butanes, etc., vol%	12.6	12.1
	100.0	100.0

Each product, therefore, has a significant volume fraction of coal liquid, which assures a fair test of ASTM specifications, and engine performance and emission testing. The constraint on the amount of DL1 or DL2 (37-37.5 vol%) is primarily due to the lower boiling range of the coal liquids in comparison to petroleum crude. Since the coal liquids have a higher proportion of naphtha, the naphtha processing section (hydrotreating/reforming) of the fixed capacity petroleum refinery limits the amount of direct coal liquids that can be processed.

3.3 Conduct Production Runs

The purpose of the production runs is twofold:

- Provide sufficient quantities of fuel blendstocks, produced from upgrading blends of coal liquids and petroleum
- Provide sufficient quantities of fuel blendstocks, produced from upgrading petroleum material (this material is required to satisfy the blending recipes)

Because the DL2 material is of a higher quality than the DL1 material, the focus of the fuel production and testing work was on DL2. The naphtha/reforming production runs were made with 42 vol% DL2 naphtha. The catalytic cracking run was made with 43 vol% DL2 heavy distillate.

LP analysis has shown that hydrotreating the DL2 light and heavy distillate fractions is unnecessary because of their high quality (high hydrogen content, low heteroatom content). In addition, hydrotreating did not improve the combustion and ignition qualities (smoke point, cetane no.) of these two cuts. For this reason, the light and heavy distillate hydrotreating production runs did not contain any coal liquids (100 % petroleum feed).

3.4 Analyze Production Run Materials and other Blendstocks

The final fuel blending recipes were based on the actual properties of the blendstocks. The property data obtained in this step was used to replace the PIMS library data. This allowed for more accurate estimates of the properties of the final fuel blends.

---

[4] C. Lowe, T. Lee, S.Tam, J. Erwin, D.S. Moulton, “Refining and End Use Study of Coal Liquids - Effect of Direct Coal Liquefaction Severity on Upgrading Operations,” Proceedings of the First Joint Power And Fuel Systems Contractors Conference, Pittsburgh, PA, July 9-11, 1996.

3.4.1 Production run materials

Table 4 summarizes the key properties for each of the diesel fuel blendstocks. Only those properties that are used to satisfy a blend specification in the PIMS model are shown. Tables 5 and 6 are similar tables for the gasoline and jet blendstocks, respectively.

3.5 Determine Fuel Blending Recipes

After the data on the properties of the various blendstocks was collected and inputed into the model, the model was rerun to determine the final blend recipes for the test fuels. Table 7 shows the blend recipe for the two gasolines, the jet, and the three diesel test fuels on a volumetric percentage basis

3.5.1 Coal Liquid Content

The estimated amount of direct coal liquid contained in each of the blended fuels is presented below.

Test Fuel	Volume % Coal Liquid
DL2 Conventional Regular Gasoline	48.8
DL2 Reformulated Premium Gasoline	40.2
DL2 Jet A	30.0
DL1 Highway Diesel	16.0
DL2 Highway Diesel	15.9
DL2 Off-Road Diesel	30.8

Note that the coal liquid content in the gasolines is higher than in the diesels. There are three primary reasons for this:

- Compared to petroleum crudes, the direct coal liquids have a lower end point and a higher proportion of naphtha material which can be converted into gasoline blendstock
- The diesel boiling range material (heavy distillate cut) of the coal liquids is catalytically cracked, primarily into gasoline blendstocks, and is not available for diesel blending
- The only coal liquid material available for diesel blending is the light distillate cut which is also used for Jet A blending

4. Summary

The production of several types of transportation fuels meeting future fuel specifications and containing significant amounts of direct coal liquids was successfully completed. The initial work involved blendstock production and property analysis. The data from these efforts was used in a linear programming model of a petroleum refinery to develop recipes based on petroleum and coal liquid blendstocks.

5. Acknowledgements

Bechtel, along with Southwest Research Institute, Amoco Corporation and the M. W. Kellogg Company, would like to express their appreciation to Shelby Rogers of DOE/FETC and the Department of Energy for their guidance and technical assistance, and for their financial support under Contract No. DE-AC22-93PC91029.

Table 1 - Option 1 LP Model, Gasoline Specifications

	Conv. regular	Reform. premium
Road octane no.	87	92
Sulfur, ppmw max	339	339
RVP, psia max[1]	8.7	-
Benzene, vol% max	1.0	1.0
Aromatics, vol% max[1]	-	-
Olefins, vol% max[1]	-	-
% off at 200 F, min	46	46
% off at 300 F min	83	83
Oxygen, wt% min.	-	2.1
Oxygen wt% max	-	2.7
Volatile organic compounds, mg/mile[2]	1378	1021
Toxic compounds, mg/mile[2]	84.8	68
Nitrogen oxides, mg/mile[2]	1346	1272

[1] No specification, but level used to estimate VOC, Toxics, and NOx per EPA Complex Model
[2] Estimated per EPA Complex Model

Table 2 - Option 1 LP Model, Jet Fuel Specifications

Max sulfur, wt%	0.1
Max aromatics, LV%	19.5
Min. percent off at 400 °F	10.0
Min. specific gravity/API	0.7927/47.0
Max. specific gravity/API	0.8397/37.0
Min. luminometer number/smoke pt	46/21

Table 3 - Option 1 LP Model, Diesel Specifications

	Off-Road Diesel	Low Sulfur Diesel
Max sulfur, wt%	0.25	0.05
Min cetane index	40	46
Min. specific gravity/API	0.8324/38.5	0.8324/38.5
Max. specific gravity/API	0.8654/32.0	0.8654/32.0
Max pour point, °F	15.8	15.8

Table 4 - Diesel Blendstock Properties

Blendstock	S.G.	S, ppm	Cetane no.	Pour pt., F
Hydrotreated kerosene	0.8063	9	45.2	-49.0
SR petroleum lt. distillate	0.8196	6010	43.0	-51.0
SR DL1 lt distillate	0.8762	230	25.0	-85.0
SR DL2 lt distillate	0.8638	13	27.8	-85.0
SR petroleum hvy distillate	0.8569	13300	49.5	-26.0
Hydrotreated hvy distillate	0.8398	6	51.4	1.4
SR DL1 hvy. distillate	0.9194	300	34.0	-15.0
SR DL2 hvy distillate	0.9139	21	34.2	-7.6
Cat diesel	0.9780	8360	17.1	-26.0
Hydrocracker diesel	0.8464	170	46.2	16.0

Table 5 - Gasoline Blendstock Properties

Blendstock	S.G.	S, ppm	Benzene, vol%	Olefins, vol%	Aromatic, vol%	% off at 200F	% off at 300F	RVP	Oxygen, wt%	(R+M)/2 octane
Cat cracker DeC_5 ovhd	0.59	0	0	29.4	0.5	100	100	19.7	0	92.5
Cat cracker DeC_5 btms	0.791	1190	1.12	7.3	45.8	30	56	2.53	0	85.35
Hydrocracker lt. naphtha	0.7675	60	4.08	1.2	28	35	100	2.77	0	87.8
Isomerate	0.6763	40	0	0	0.4	98	100	14.82	0	87.8
Normal butane	0.5849	0	0	0	0	100	100	51.6	0	91.7
Reformate	0.8117	0	1.7	1	53.8	8	63	1.95	0	85.8
MTBE	0.746	0	0	0	0	43	88	8.7	18.2	110
Alkylate	0.6972	70	0.12	0	0	37	92	6.76	0	90.4

Table 6 - Jet A Blendstock Properties

Blendstock	S.G.	S, ppm	Aromatic, vol%	% off at 400 F	Smoke pt, mm
Hydrotreated kerosene	0.8063	9.3	14.3	50	24.7
SR petroleum lt. distillate	0.8196	6010	21.1	32.5	20
SR DL1 lt distillate	0.8762	230	58.7	14	9.5
SR DL2 lt distillate	0.8638	13.1	24	26.3	14.5

Table 7 - Fuel Blending Recipes (vol%)

Blendstock	DL2 conv. regular gasoline	DL2 reform. premium gasoline	DL2 Jet A	DL1 highway diesel	DL2 off-road diesel	DL2 highway diesel
Cat cracker DeC_5 ovhd	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Cat cracker DeC_5 btms	26.7%	23.2%	0.0%	0.0%	0.0%	0.0%
Hydrocracker lt. naphtha	0.0%	2.3%	0.0%	0.0%	0.0%	0.0%
Isomerate	20.9%	1.1%	0.0%	0.0%	0.0%	0.0%
Normal butane	5.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Reformate	41.1%	4.1%	0.0%	0.0%	0.0%	0.0%
MTBE	4.1%	11.3%	0.0%	0.0%	0.0%	0.0%
Alkylate	2.3%	58.1%	0.0%	0.0%	0.0%	0.0%
Hydrotreated kerosene	0.0%	0.0%	53.4%	5.6%	0.0%	12.4%
SR petroleum lt. distillate	0.0%	0.0%	16.6%	6.3%	28.0%	6.9%
SR DL1 lt distillate	0.0%	0.0%	0.0%	16.0%	0.0%	0.0%
SR DL2 lt distillate	0.0%	0.0%	30.0%	0.0%	7.1%	15.9%
SR petroleum hvy distillate	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Hydrotreated hvy distillate	0.0%	0.0%	0.0%	72.1%	31.2%	64.8%
SR DL1 hvy. distillate	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
SR DL2 hvy distillate	0.0%	0.0%	0.0%	0.0%	15.5%	0.0%
Cat diesel	0.0%	0.0%	0.0%	0.0%	8.1%	0.0%
Hydrocracker diesel	0.0%	0.0%	0.0%	0.0%	10.0%	0.0%
Total	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%